Quality of Prediction Analysis in Pareto Solutions

Nuno Costa and João Lourenço

Abstract— **In practice, a unique solution is selected from a representative set of optimal solutions for solving a multiresponse optimization problem. However, the reproducibility of these solutions has been ignored so far, which may jeopardize the usefulness of some optimal solutions. Here, it is shown that the quality of prediction of each optimal solution is different, which may justify the lack of the reproducibility of Pareto solutions in some real-life situations. This means that the decision-maker has to take into account the solutions quality of prediction when he/she selects a solution. For this purpose, a metric to assess the solutions quality of prediction is suggested. A bi-objective problem is used as example and results displayed graphically.**

Index Terms— **Compromise, Conflict, Multiresponse, Optimal, Optimization, Variance.**

I. Introduction

INDUSTRIAL problems are, by nature, multidimensional so the optimization of multiobjective (multiresponse) problems has been an active research field. Conflicting responses are usual in these problems and their simultaneous optimization has been recommended and an often used practice to generate compromise solutions. A desired condition for any candidate solution to multiresponse problems is that the solution is non-dominated. This means that better values for one or more responses cannot be achieved in one solution without degrading the value of, at least, another response.

A representative set of optimal or non-dominated solutions constitutes the so-called Pareto front, and provides the most favorable alternative choices for solving a multiresponse optimization problem (MROp). However, assuming that the Pareto front was appropriately generated, the decision-maker faces another issue: how to choose an optimal solution from the generated set. This is not a trivial task, because the reproducibility of optimal solutions cannot be ignored by the decision-maker. In fact, there is no guarantee that product or process performs as expected when is run at a chosen input variable location due to the natural process variability and the estimated solutions uncertainty. This means that the quality of prediction for each optimal solution has to be assessed and considered in the decision process, which has been ignored so far. Therefore, the objective of this manuscript is to introduce a metric to assess the solutions quality of prediction and help the decision-maker in making a more informed decision in the solution selection process.

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II. Pareto Optimality - Dominance Relation

A MROp can be defined as follows:

$$\begin{gathered}\text{Minimize } f(\mathbf{r}, \mathrm{M}) \\ \mathrm{x} \\ \text{subject to} \\ \mathbf{g}(\mathbf{x}, \mathbf{b}) \leq 0 \\ \mathbf{h}(\mathbf{x}, \mathbf{b}) = 0 \\ \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u\end{gathered} \tag{1}$$

where f is a scalar valued function, M represents the set of user-specified or preference parameters (weights, priorities, shape factors, …), and $\mathbf{r}$ is the vector of responses $(r = 1,..., p)$. The called design parameters, which are not controlled by the *DM*, are denoted by $\mathbf{b}$. Design or input variables, denoted by vector $\mathbf{x}$, with lower bound $\mathbf{x}_l$ and upper bound $\mathbf{x}_u$. Constraints are represented by $\mathbf{g}(\mathbf{x}, \mathbf{b})$ and $\mathbf{h}(\mathbf{x}, \mathbf{b})$.

In contrast to single response optimization problems, where the optimal solution is defined easily, for a MROp a solution is more of a concept than a definition [1]. In practice, a compromise solution has to be selected, because the utopia point (the variables setting that yields a solution with all responses at their target value) for formulation (1) cannot be achieved.

A predominant concept in defining a non-dominated solution is that of Pareto optimality. For a minimization problem like that formulated in Eq. (1), a solution (a vector of responses; r_1) dominates another one (r_2), and is Pareto optimal, if both the following conditions are true:

--First, the value of any response in r_1 is no worse (is lower or equal) than those of r_2;

--Second, the value of at least one response in r_1 is strictly better (is lower) than those of r_2.

Pareto frontiers can be displayed graphically only for problems with two or three responses, and consensus on what qualities a representation of the non-dominated set should possess do not exist. According to [2], quality measures that have been proposed and may be useful to this end are the following: 1- measures of cardinality (which refer to the number of points in a representation); 2- coverage (which refer to the regions of the outcome set that are represented); 3- spacing (which refer to the distance between points in the representation). Hybrid measures which overlap the above three categories have been also

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introduced in the literature. An example is the hypervolume measure, a well-established indicator of the front's quality [3-4].

A representative set of non-dominated solutions for solving a MROp is helpful, since it provides a broad overview of alternative solutions. However, in practice, only one solution is selected. This leads to a critical question: which optimal solution should be chosen?

III. Reproducibility of Non-dominated Solutions

A discrete representation of a Pareto frontier (a collection of solutions distributed along the Pareto front that provides a finite and manageable alternative set of solutions to the decision-maker) is, in general, sufficient for selecting a solution for a MROp. Majority of the literature has focused on how to find the PF with its most promising choices without providing more insights on how to proceed from those choices to a final decision [5]. However, it is important to be aware that some Pareto solutions may lead to operation conditions more hazardous, more costly or more difficult to implement and control than others. In fact, the responses' quality of prediction is not the same for all the Pareto solutions and, if it is ignored, can potentially lead to suboptimal choices and the selected solution may yield, in practice, unexpected results. To minimize the gap between the theoretical and practical results, the decision-maker must estimate the solutions quality of prediction. For this purpose, and assuming that Ordinary Least Squares regression technique is used to fit models to each response, the proposed metric is

$$QoP = trace\left[\varphi \sum_{\hat{y}} (\mathrm{x}^*)\right] \tag{2}$$

where φ is a matrix whose elements are $\varphi_{ii} = 1/(U_i - L_i)^2$ and $\varphi_{ij} = 1/(U_i - L_i)(U_j - L_j)$ for $i \neq j$, with $i, j = 1, 2, ..., n$, and $\sum_{\hat{y}}(\mathrm{x}^*)$ represents the variance-covariance matrix of the n estimated responses at optimal location x*. When all the models fitted to responses have the same regressors, one can write

$$\sum_{\hat{y}}(\mathrm{x}^*) = \mathrm{x}^{*T}(X'X)^{-1}\mathrm{x}^*\hat{\Sigma} \tag{3}$$

where X is the model matrix, $\hat{\Sigma} = \hat{e}_i^T \hat{e}_j / N$, $\hat{e}$ represents the estimated residuals (difference between the observed response value and the corresponding estimated value) and N is the number of experimental observations [6]. If the SUR technique is used, the reader is referred to [7] where a variant of the QoP metric is defined and illustrated.

IV. Examples

The objective of this example is to determine the settings for reaction time (x_1), reaction temperature (x_2), and amount of catalyst (x_3) to maximize the conversion (y_1) of a polymer and achieve a target value for the thermal activity (y_2). A central composite design with four center points was run and the (mean) models fitted to responses are

$$\hat{\mu}_1 = 81.0943 + 1.0290\,x_1 + 4.0426\,x_2 + 6.2060\,x_3 - 1.8377\,x_1^2 + 2.9455\,x_2^2 - 5.2036\,x_3^2 + 2.1250\,x_1x_2 + 11.3750\,x_1x_3 - 3.8750\,x_2x_3$$

$$\hat{\mu}_2 = 59.8505 + 3.5855\,x_1 + 0.2547\,x_2 + 2.2312\,x_3 + 0.8360\,x_1^2 + 0.0742\,x_2^2 + 0.0565\,x_3^2 - 0.3875\,x_1x_2 - 0.0375\,x_1x_3 + 0.3125\,x_2x_3$$

The range values for y_1 and y_2 are [80, 100] and [55, 60], respectively. Assuming that y_1 is a LTB-type response (the estimated response value is expected to be equal or larger than an upper bound), the target value is set equal to 100; y_2 is a NTB-type response (its estimated response value is expected to be equal to a target value) and the target value is set equal to 57.5. The constraints for the input variables are $-1.682 \leq x_i \leq 1.682\,(i = 1, 2, 3)$.

Figure 1 displays the Pareto front generated with the compromise programming-based criterion proposed by [8], varying the shape factor $1 \leq \omega_i \leq 12$ in increments of one unit, using a SQP algorithm. This example deals with the optimization of two responses so it was possible to display the Pareto frontier graphically, and one can see that responses are in conflict: when $\hat{\mu}_1$ increases, $\hat{\mu}_2$ deviates from target and vice-versa.

Figures 2 shows that choosing a solution based on technical, economic or decision-maker preferences may not produce the expected results in practice, because the solutions quality of prediction is not homogeneous. In this example, QoP value ranges from 6.5 to 25 units. This values range is not as small as desired, and may lead to criticisms on the time and cost spent in the study and skepticism on the use (or more widespread use) of statistically-based approaches and tools to solve industrial problems as well as attacking some challenging and exciting real problems arising today [9].

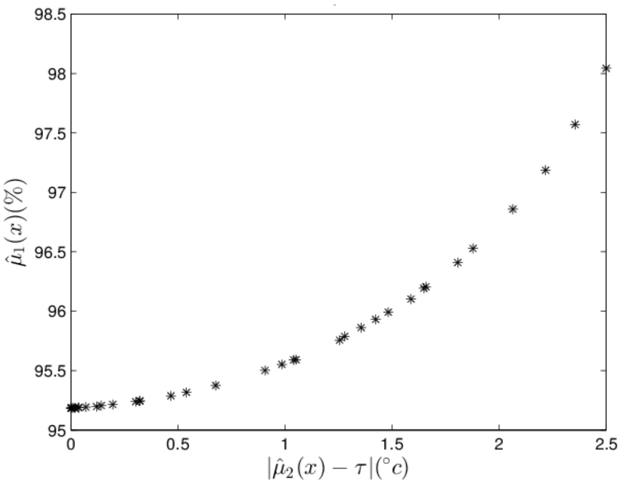

Figure 1 – Pareto front

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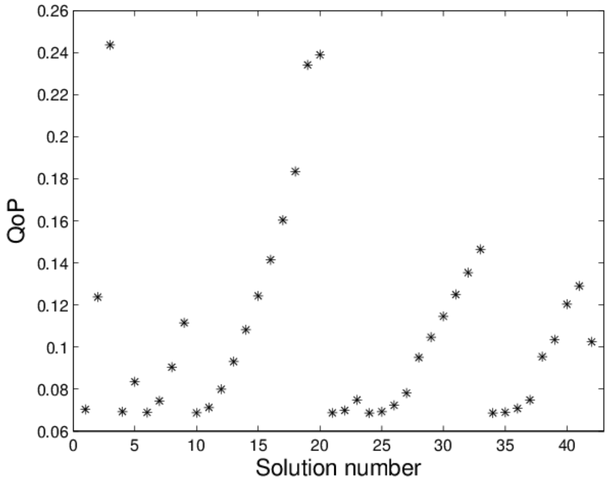

Figure 2 – Quality of Predictions

V. Results Discussion

A compromise solution to solve a MROp must be selected among those of the Pareto front. However, those solutions may not yield the expected practical result if the quality of prediction value of selected optimal solution is (excessively) high. The QoP values can be displayed graphically for problems with two responses, such as Figure 2 shows, and may help the decision-maker in making a more informed optimal solution selection. The optimal solution selection is more complicated and Pareto front visualization impossible for more than four responses so alternative tools such as tabular lists are necessary to highlight more favorable solutions in a more effective manner. Nevertheless, the decision-maker needs always to balance the conflict between responses' priority and responses' quality of prediction. For example, in the problem considered here, if priority is setting $\hat{\mu}_2$ on target value ($\hat{\mu}_2 = \tau$ see Figure 1), one can see from Figure 2 that the first solution, as well as solutions slightly deviated from target ($\hat{\mu}_2 \neq \tau$), as instance the solutions number 6 and 10, can be a good choice. If priority is setting $\hat{\mu}_1$ on target value, Figure 2 shows that QoP value is undesirably higher for solution number 42 (the solution with the highest $\hat{\mu}_1$ value) than for other optimal solutions, as instance, the thirty-fourth and thirty-fifth solutions, though their $\hat{\mu}_1$ value is slightly worst.

These results confirm that a compromise is necessary to select a solution for MROp and show that information about solutions reproducibility (QoP value) cannot be ignored. In fact, the QoP value for some responses is undesirably high and likely lead to less favorable results in practice. Confirmatory runs can help in the decision-making process. Nevertheless, the decision-maker must be aware that solutions whose response values are slightly deviated from target and QoP is lower can be effective alternatives for solving MROp and must be tested in practice.

VI. Conclusions and Future Work

This work investigates the Pareto front solutions quality, and shows that quality of prediction value is different for most Pareto front solutions. From a theoretical point of view, it is desirable to select Pareto solutions with the lowest quality of prediction value. However, this may not be possible due to the conflict between responses priority and solutions' quality of prediction. In fact, the quality of prediction value may be undesirably higher for response values of interest. Thus, in practice, a compromise between technical and economic considerations will dictate the final decision about the most favorable solution.

To help the decision-maker in making more informed decisions, future work shall investigate the impact of models coefficient uncertainty in Pareto fronts. Optimal solutions built on the worst-case estimated responses must be generated and other metric(s) developed to evaluate optimal solutions.

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References

[1] R. Marler, and J. Arora, "Survey of multi-objective optimization methods for engineering", *Structural Multidisciplinary Optimization*, vol. 26, no. 1, pp. 369-395, 2004.
[2] S. Faulkenberg, and M. Wiecek, "On the quality of discrete representations in multiple objective programming", *Optimization and Engineering*, vol. 11, no. 3, pp. 423-440, 2010.
[3] Y. Cao, B. Smucker, and T. Robinson, "On using the hypervolume indicator to compare Pareto fronts: Applications to multi-criteria optimal experimental design", *Journal of Statistical Planning and Inference*, vol. 160, no. 8, pp. 60-74, 2015.
[4] L. Lu, and C. Anderson-Cook, "Adapting the hypervolume quality indicator to quantify trade-offs and search efficiency for multiple criteria decision making using Pareto fronts", *Quality and Reliability Engineering International*, vol. 29, no. 8, pp. 1117-1133, 2012.
[5] J. Chapman, L. Lu, and C. Anderson-Cook, "Impact of response variability on Pareto front optimization", *Statistical Analysis and Data Mining: The ASA Data Science Journal*, vol. 8, no. 5-6, pp. 314-328, 2015.
[6] G. Vining, "A compromise approach to multiresponse optimization", *Journal of Quality Technology*, vol. 30, no. 2, pp. 309-313, 1998.
[7] N. Costa, J. Lourenço, and Z. Pereira, "Responses Modeling and Optimization Criteria Impact on the Optimization of Multiple Quality Characteristics", *Computers & Industrial Engineering*, vol. 62, no. 4, pp. 972-935, 2012.
[8] N. Costa, and Z. Pereira, "Multiple response optimization: a global criterion-based method", *Journal of Chemometrics*, vol. 24, no. 6, pp. 333-342, 2010.
[9] D. Steinberg, "Industrial statistics: The challenges and the research", *Quality Engineering*, vol. 28, no. 1, pp. 45-59, 2016.